Optimized AgCuSe-Cys nanocrystals as amplifiers for SEIRA Detection of Pharmaceuticals

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Semiconductor nanocrystals (NCs), also known as quantum dots, have attracted significant attention due to their broad range of applications, including environmental monitoring, sensing, and biomedicine [1]. However, many conventional NCs contain toxic elements such as cadmium or lead and are commonly synthesized under harsh conditions involving high temperatures, organic solvents, and hazardous reagents [2]. In this context, Cu- and Ag-based NCs have emerged as promising alternatives, combining attractive optical properties with lower toxicity, although their synthesis still frequently depends on non-aqueous media and energy-intensive conditions [3].

The controlled synthesis of semiconductor NCs requires a detailed understanding of how experimental parameters influence their formation, composition, and photophysical properties [4]. In multicomponent systems, where variables are often interdependent, traditional one-factor-at-a-time approaches are inefficient and inadequate for robust optimization. In this work, a multivariate experimental design was applied to optimize the aqueous synthesis of cysteine-stabilized AgCuSe nanocrystals (AgCuSe-Cys), aiming to evaluate the influence of synthesis parameters on their fluorescence behavior.

A three-level factorial design comprising 27 experiments was employed to investigate the combined effects of Se precursor, Cys (stabilizing agent), and ascorbic acid (reducing agent) concentrations on fluorescence intensity. The total metal concentration was kept constant to isolate the effects of the selected variables. All syntheses were performed under controlled conditions (pH 8.0, 70 °C) in randomized order to minimize systematic bias, and samples were analyzed one week after preparation to ensure colloidal stabilization.

ANOVA results demonstrated that Se precursor and Cys concentrations significantly affected fluorescence intensity, whereas ascorbic acid showed no statistically significant influence. Pareto analysis revealed that Cys concentration contributed positively to fluorescence enhancement, with higher concentrations leading to increased emission intensity, while selenium precursor concentration exhibited a negative effect, with lower levels favoring stronger fluorescence.

Overall, this study highlights the effectiveness of multivariate experimental design as a rational strategy for optimizing the aqueous synthesis of AgCuSe-Cys NCs. In addition, preliminary results indicate that the optimized NCs have potential for future application as sensing platforms in surface-enhanced infrared absorption (SEIRA) spectroscopy for detecting pharmaceutical contaminants in water.

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